

09/ 939,883

STRUCTURE FILE UPDATES: 14 DEC 2004 HIGHEST RN 797749-23-6  
DICTIONARY FILE UPDATES: 14 DEC 2004 HIGHEST RN 797749-23-6

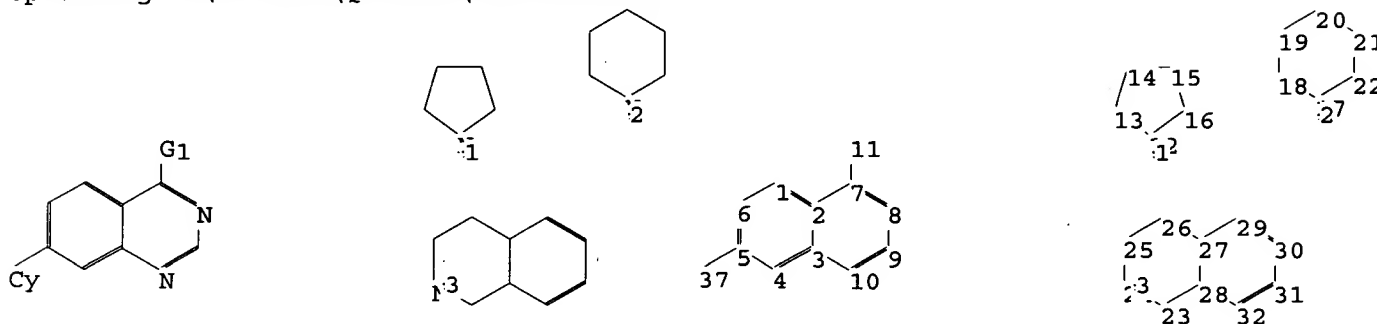
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>  
Uploading C:\STNEXP4\QUERIES\09939883.str



chain nodes :

11 37

ring nodes :

1 2 3 4 5 6 7 8 9 10 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26  
27 28 29 30 31 32

chain bonds :

5-37 7-11

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10 12-13 12-16 13-14 14-15  
15-16 17-18 17-22 18-19 19-20 20-21 21-22 23-24 23-28 24-25 25-26 26-27 27-28  
27-29 28-32 29-30 30-31 31-32

exact/norm bonds :

5-37 7-11 27-28 27-29 28-32 29-30 30-31 31-32

exact bonds :

12-13 12-16 13-14 14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22 23-24 23-28  
24-25 25-26 26-27

normalized bonds :

1-2 1-6 2-3 2-7 3-4 3-10 4-5 5-6 7-8 8-9 9-10

isolated ring systems :

containing 1 : 12 : 17 : 23 :

G1:[\*1],[\*2],[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS  
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom  
22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
32:Atom 37:Atom

Element Count :

Node 37: Limited

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C,C4-8

S,S0-1

N,N0-2

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 11:22:03 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3187 TO ITERATE

100.0% PROCESSED 3187 ITERATIONS

40 ANSWERS

SEARCH TIME: 00.00.01

L2 40 SEA SSS FUL L1

=> file caplus

FILE 'CAPLUS' ENTERED AT 11:22:08 ON 16 DEC 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 16 Dec 2004 VOL 141 ISS 25

FILE LAST UPDATED: 15 Dec 2004 (20041215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l2

L3 3 L2

=> d l3 1- ibib abs hitstr

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

09/ 939,883

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:185085 CAPLUS

DOCUMENT NUMBER: 136:247596

TITLE: Preparation of 7-aryl-4-(1-azacycloalkyl)quin(az)olines and analogs as NPY receptor antagonists

INVENTOR(S): Breu, Volker; Dautzenberg, Frank; Guerry, Philippe; Nettekoven, Matthias Heinrich; Pflieger, Philippe

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: PCT Int. Appl., 62 pp.

CODEN: PIXXD2

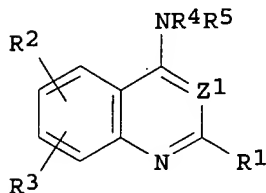
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002020488	A2	20020314	WO 2001-EP10014	20010830
WO 2002020488	A3	20020516		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2002052356	A1	20020502	US 2001-939883	20010827
CA 2420703	AA	20020314	CA 2001-2420703	20010830
AU 2002010474	A5	20020322	AU 2002-10474	20010830
BR 2001013710	A	20030603	BR 2001-13710	20010830
EP 1318981	A2	20030618	EP 2001-978324	20010830
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2004508357	T2	20040318	JP 2002-525110	20010830
PRIORITY APPLN. INFO.:			EP 2000-119262	A 20000906
			WO 2001-EP10014	W 20010830
OTHER SOURCE(S):	MARPAT 136:247596			
GI				



AB Title compds. [I; R1 = (cyclo)alkyl, CF3, aralkyl; R2 = H, halo, alkyl, alkoxy, etc.; R3 = (hetero)aryl; NR4R5 = (un)substituted heterocyclyl; Z1 = CH or N] were prepared. Thus, 4-chloro-7-iodo-2-methylquinoline was aminated by pyrrolidine and the product arylated by 3-ClC6H4B(OH)2 to give I [R1 = Me, R2 = H, R3 = 7-(3-chlorophenyl), R4R5 = (CH2)4, Z1 = CH]. Data for biol. activity of I were given.

IT 403849-51-4P 403849-52-5P 403849-53-6P  
403849-54-7P 403849-55-8P 403849-56-9P  
403849-57-0P 403849-58-1P 403849-60-5P  
403849-62-7P 403849-64-9P 403849-66-1P

*pregnant version*

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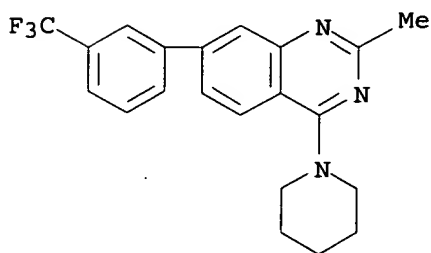
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403849-76-3P 403849-80-9P 403849-82-1P  
403849-84-3P 403849-86-5P 403849-88-7P  
403853-06-5P 403853-08-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU  
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
(Uses)

(preparation of 7-aryl-4-(1-azacycloalkyl)quin(az)olines and analogs as NPY  
receptor antagonists)

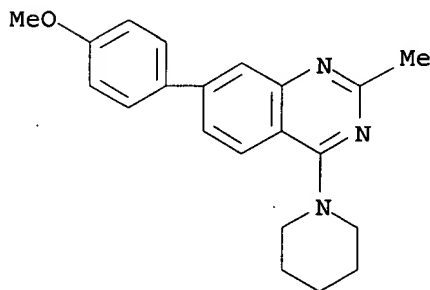
RN 403849-51-4 CAPLUS

CN Quinazoline, 2-methyl-4-(1-piperidinyl)-7-[3-(trifluoromethyl)phenyl]-  
(9CI) (CA INDEX NAME)



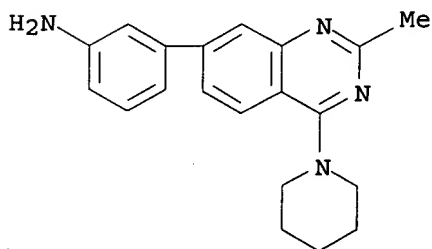
RN 403849-52-5 CAPLUS

CN Quinazoline, 7-(4-methoxyphenyl)-2-methyl-4-(1-piperidinyl)- (9CI) (CA  
INDEX NAME)



RN 403849-53-6 CAPLUS

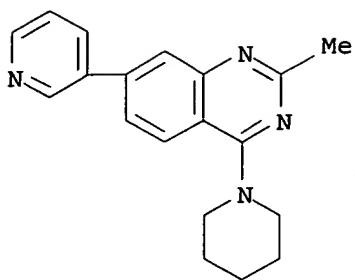
CN Benzenamine, 3-[2-methyl-4-(1-piperidinyl)-7-quinazolinyl]- (9CI) (CA  
INDEX NAME)



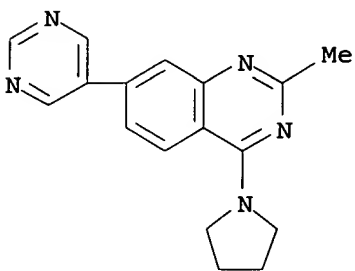
RN 403849-54-7 CAPLUS

CN Quinazoline, 2-methyl-4-(1-piperidinyl)-7-(3-pyridinyl)- (9CI) (CA INDEX  
NAME)

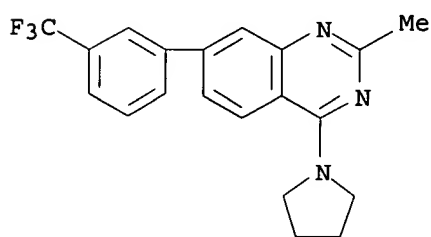
09/ 939,883



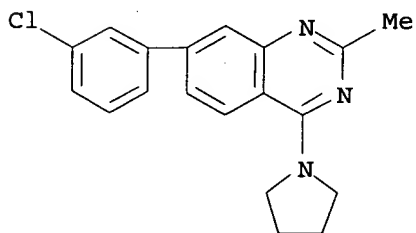
RN 403849-55-8 CAPLUS  
CN Quinazoline, 2-methyl-7-(5-pyrimidinyl)-4-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 403849-56-9 CAPLUS  
CN Quinazoline, 2-methyl-4-(1-pyrrolidinyl)-7-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

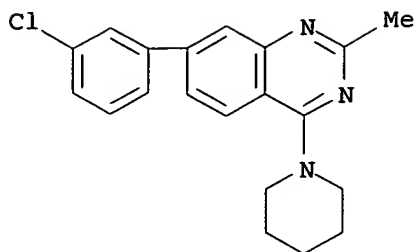


RN 403849-57-0 CAPLUS  
CN Quinazoline, 7-(3-chlorophenyl)-2-methyl-4-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

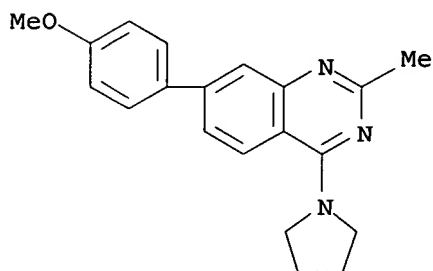


RN 403849-58-1 CAPLUS  
CN Quinazoline, 7-(3-chlorophenyl)-2-methyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)

09/ 939,883



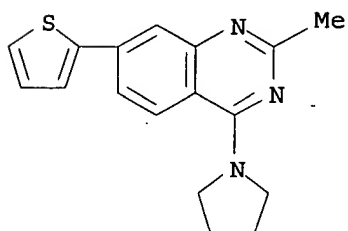
RN 403849-60-5 CAPLUS  
CN Quinazoline, 7-(4-methoxyphenyl)-2-methyl-4-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)



RN 403849-62-7 CAPLUS  
CN Formic acid, compd. with 2-methyl-4-(1-pyrrolidinyl)-7-(2-thienyl)quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-61-6  
CMF C17 H17 N3 S



CM 2

CRN 64-18-6  
CMF C H2 O2

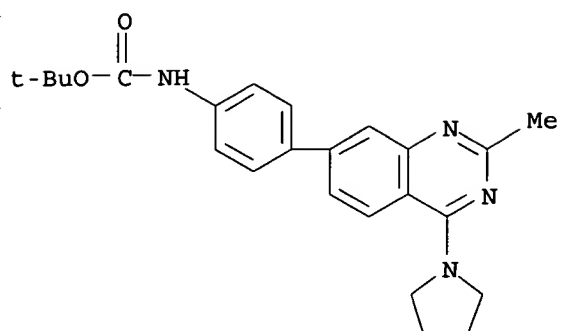
O=CH-OH

RN 403849-64-9 CAPLUS  
CN Carbamic acid, [4-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]phenyl]-, 1,1-dimethylethyl ester, monoformate (9CI) (CA INDEX NAME)

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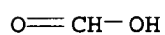
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CRN 403849-63-8  
CMF C24 H28 N4 O2

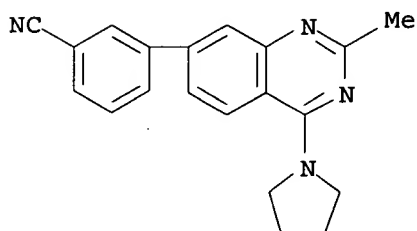


CM 2

CRN 64-18-6  
CMF C H2 O2



RN 403849-66-1 CAPLUS  
CN Benzonitrile, 3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]- (9CI) (CA INDEX NAME)

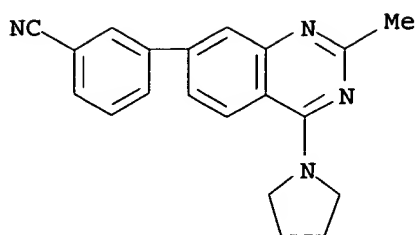


RN 403849-67-2 CAPLUS  
CN Formic acid, compd. with 3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]benzonitrile (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-66-1  
CMF C20 H18 N4

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CM 2

CRN 64-18-6

CMF C H2 O2

O=CH-OH

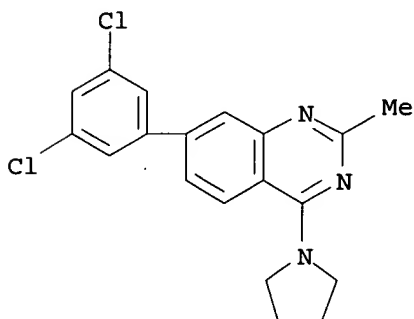
RN 403849-69-4 CAPLUS

CN Formic acid, compd. with 7-(3,5-dichlorophenyl)-2-methyl-4-(1-pyrrolidinyl)quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-68-3

CMF C19 H17 Cl2 N3



CM 2

CRN 64-18-6

CMF C H2 O2

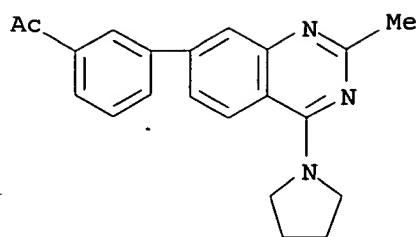
O=CH-OH

RN 403849-70-7 CAPLUS

CN Ethanone, 1-[3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]phenyl]- (9CI)  
(CA INDEX NAME)



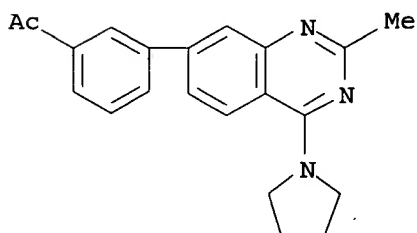
09/ 939,883



RN 403849-71-8 CAPLUS  
CN Formic acid, compd. with 1-[3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]phenyl]ethanone (1:1) (9CI) (CA INDEX NAME)

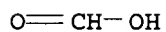
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CRN 403849-70-7  
CMF C21 H21 N3 O



CM 2

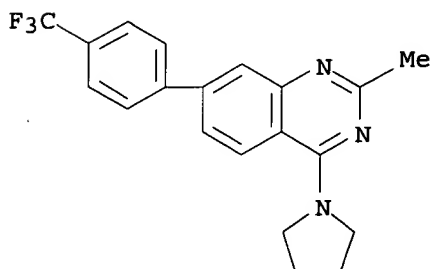
CRN 64-18-6  
CMF C H2 O2



RN 403849-73-0 CAPLUS  
CN Formic acid, compd. with 2-methyl-4-(1-pyrrolidinyl)-7-[4-(trifluoromethyl)phenyl]quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-72-9  
CMF C20 H18 F3 N3



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CM 2

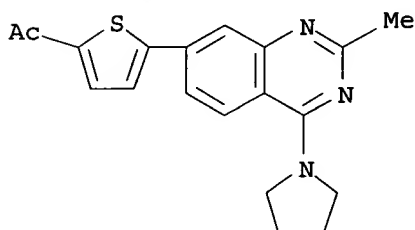
CRN 64-18-6  
CMF C H2 O2

O=CH-OH

RN 403849-75-2 CAPLUS  
CN Formic acid, compd. with 1-[5-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]-2-thienyl]ethanone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-74-1  
CMF C19 H19 N3 O S

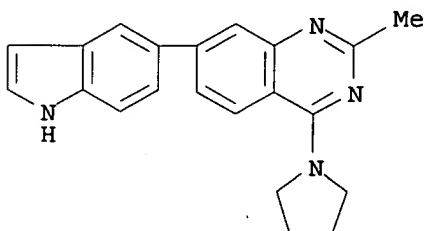


CM 2

CRN 64-18-6  
CMF C H2 O2

O=CH-OH

RN 403849-76-3 CAPLUS  
CN Quinazoline, 7-(1H-indol-5-yl)-2-methyl-4-(1-pyrrolidinyl)- (9CI) (CA INDEX NAME)

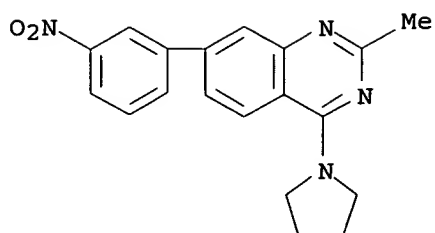


RN 403849-80-9 CAPLUS  
CN Formic acid, compd. with 2-methyl-7-(3-nitrophenyl)-4-(1-pyrrolidinyl)quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-79-6  
CMF C19 H18 N4 O2

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CM 2

CRN 64-18-6

CMF C H2 O2

O=CH-OH

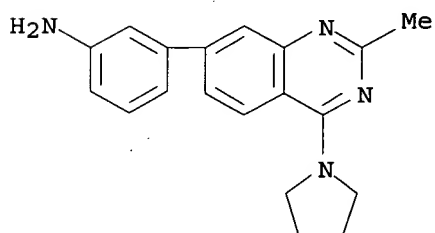
RN 403849-82-1 CAPLUS

CN Formic acid, compd. with 3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]benzenamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-81-0

CMF C19 H20 N4



CM 2

CRN 64-18-6

CMF C H2 O2

O=CH-OH

RN 403849-84-3 CAPLUS

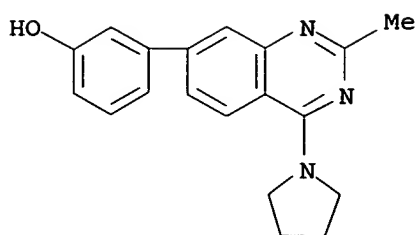
CN Formic acid, compd. with 3-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]phenol (1:1) (9CI) (CA INDEX NAME)

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CRN 403849-83-2

CMF C19 H19 N3 O

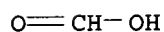
09/ 939,883



CM 2

CRN 64-18-6

CMF C H2 O2



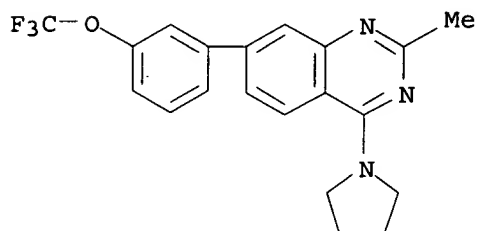
RN 403849-86-5 CAPLUS

CN Formic acid, compd. with 2-methyl-4-(1-pyrrolidinyl)-7-[3-(trifluoromethoxy)phenyl]quinazoline (1:1) (9CI) (CA INDEX NAME)

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CRN 403849-85-4

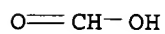
CMF C20 H18 F3 N3 O



CM 2

CRN 64-18-6

CMF C H2 O2



RN 403849-88-7 CAPLUS

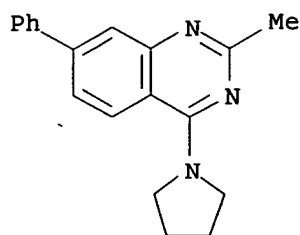
CN Formic acid, compd. with 2-methyl-7-phenyl-4-(1-pyrrolidinyl)quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403849-87-6

CMF C19 H19 N3

09/ 939,883



CM 2

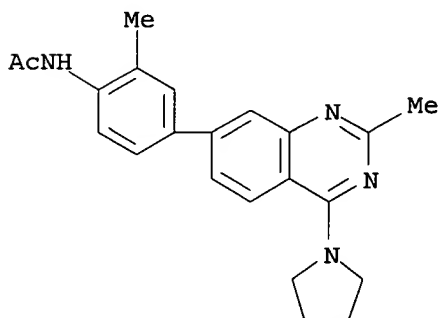
CRN 64-18-6  
CMF C H2 O2



RN 403853-06-5 CAPLUS  
CN Formic acid, compd. with N-[2-methyl-4-[2-methyl-4-(1-pyrrolidinyl)-7-quinazolinyl]phenyl]acetamide (1:1) (9CI) (CA INDEX NAME)

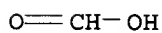
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CRN 403853-05-4  
CMF C22 H24 N4 O



CM 2

CRN 64-18-6  
CMF C H2 O2

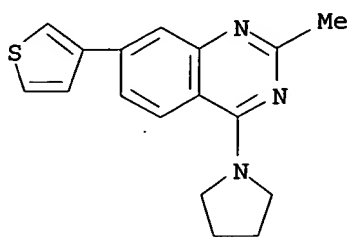


RN 403853-08-7 CAPLUS  
CN Formic acid, compd. with 2-methyl-4-(1-pyrrolidinyl)-7-(3-thienyl)quinazoline (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 403853-07-6  
CMF C17 H17 N3 S

09/ 939,883



CM 2

CRN 64-18-6

CMF C H2 O2

O=CH-OH

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:505445 CAPLUS

DOCUMENT NUMBER: 115:105445

TITLE: Studies on cardiotonic agents. VII. Potent cardiotonic agent KF15232 with myofibrillar calcium sensitizing effect

AUTHOR(S): Nomoto, Yuji; Takai, Haruki; Ohno, Tetsuji; Kubo, Kazuhiro

CORPORATE SOURCE: Pharm. Res. Lab., Fuji, Kyowa Hakko Kogyo Co., Ltd., Shizuoka, 411, Japan

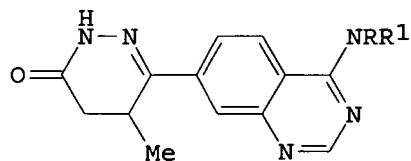
SOURCE: Chemical & Pharmaceutical Bulletin (1991), 39(4), 900-10

CODEN: CPBTAL; ISSN: 0009-2363

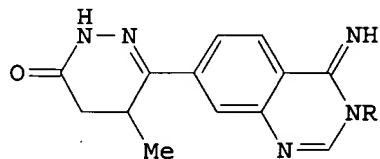
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I, R=H, alkyl, cycloalkyl, etc., R<sup>1</sup>=H, RR<sup>1</sup>=alkylene



II, R=NH<sub>2</sub>, alkyl, Ph, etc.

AB A series of novel 4,5-dihydro-5-methyl-6-(4-substituted

7-quinazolinyl)-3-(2H)pyridazinones (I) was synthesized and examined for cardiotoxic activity in anesthetized dogs. The 4-substituted aminoquinazolines generally showed potent and long-lasting inotropic activity. Fall in the activity was observed on the introduction of substituent at the 2-position of the quinazoline ring. The 3-substituted 4-(3H)quinazolinimines (II) generally exhibited weak activity. Ca<sup>2+</sup> sensitizing effect of the 4-substituted amino derivs. was also examined in chemical skinned fiber from papillary muscle of guinea pig. The alkylamine derivs. exhibited small sensitizing effect, while the benzylamino derivs. exhibited large effect. Among them, KF15232 (Ix) was found to have the most potent cardiotoxic and Ca<sup>2+</sup> sensitizing activities.

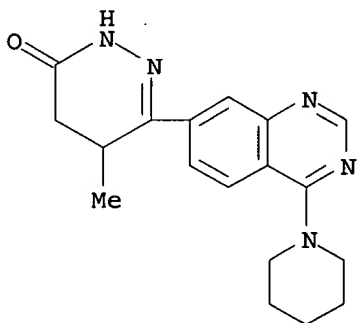
IT 124294-61-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and cardiotoxic activity of, structure in relation to)

RN 124294-61-7 CAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-5-methyl-6-[4-(1-piperidinyl)-7-quinazolinyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:21004 CAPLUS

DOCUMENT NUMBER: 112:21004

TITLE: Preparation, testing, and formulation of 4,5-dihydro-6-aryl-2-oxopyridazines as cardiotonics and antihypertensives

INVENTOR(S): Nomoto, Yuji; Takai, Haruki; Ohno, Tetsuji; Kubo, Kazuhiro

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 48 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

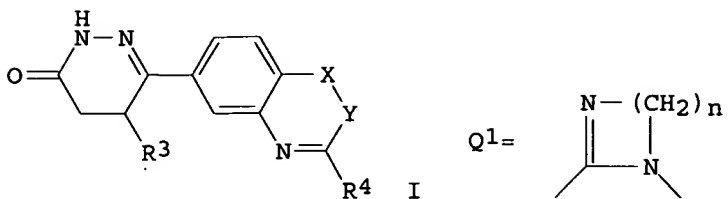
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 326307	A2	19890802	EP 1989-300611	19890123
EP 326307	A3	19900912		
EP 326307	B1	19940817		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
JP 02022274	A2	19900125	JP 1989-7055	19890113
US 5063227	A	19911105	US 1990-462914	19900111
PRIORITY APPLN. INFO.:			JP 1988-13301	A 19880123
			US 1989-297440	B1 19890117

GI



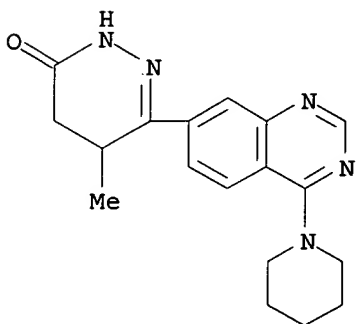
AB The title compds. [I; R1,R2 = H, (substituted) alkyl, alkenyl, aralkyl, aryl, amino, alkoxy, carbonylamino, pyridylalkyl; NR1R2 = heterocyclyl; R3 = H, alkyl; R4 = H, SH, OH, (substituted) alkyl, alkylthio, alkoxy, NR1R2; R5 = H, alkyl, NR1R2; X - Y = CH2NH, R5C:N, Q1, etc.; n = 2,3], useful as cardiotonics and antihypertensives, were prepared. Thus, 3-(4-bromo-3-nitrobenzoyl)butyric acid (prepn given) was cyclocondensed with N2H4 in HOAc to give 100% 6-(4-bromo-3-nitrophenyl)-4,5-dihydro-5-methyl-3(2H)pyridazinone. The latter was cyanated with CuCN in DMF (44%) followed by reduction with SnCl2/HCl to give 87% 6-(3-amino-4-cyanophenyl)-4,5-dihydro-5-methyl-3(2H)pyridazinone. This was condensed with (EtO)3CH to give 24% of the 3-ethoxymethyleneamino derivative, which was cyclized in MeOH containing MeNH2 to give the corresponding pyridazinone, which was heated with 2N NaOH to give 76% 4,5-dihydro-5-methyl-6-(4-methylaminoquinazolin-7-yl)-3(2H)pyridazinone. The latter at 0.03 mg/kg i.v. in dogs increased myocardiac contractility with a  $\Delta dp/dt$  of 78.3%.

IT 124294-61-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as cardiotonic and antihypertensive)

RN 124294-61-7 CAPLUS

CN 3(2H)-Pyridazinone, 4,5-dihydro-5-methyl-6-[4-(1-piperidinyl)-7-quinazolinyl]- (9CI) (CA INDEX NAME)



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(FILE 'HOME' ENTERED AT 11:21:31 ON 16 DEC 2004)

FILE 'REGISTRY' ENTERED AT 11:21:42 ON 16 DEC 2004

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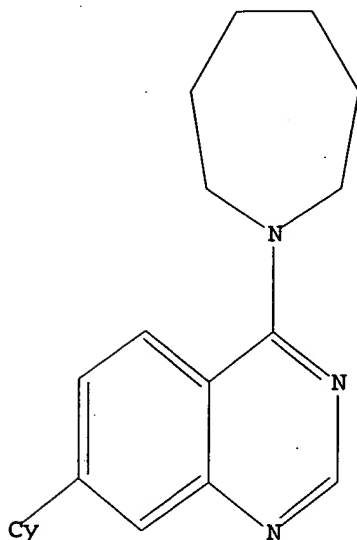
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Structure attributes must be viewed using STN Express query preparation.

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FULL SCREEN SEARCH COMPLETED - 221 TO ITERATE

100.0% PROCESSED 221 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

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FILE COVERS 1907 - 16 Dec 2004 VOL 141 ISS 25